

STIC Search Report

EIC 1700

STIC Database Tracking Number: 223265

TO: Ben Sackey
Location: Remsen 5b31
Art Unit : 1624
May 3, 2007
Phone: 571-272-0704
Serial Number: 10 / 751387

From: Jan Delaval

Location: EIC 1700
Remsen 4a30
Phone: 571-272-2504
jan.delaval@uspto.gov

Search Notes

FOR OFFICIAL USE ONLY

Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: BEN SA CKEY Examiner #: 73489 Date: 4/27/07
Art Unit: 1624 Phone Number: 2-0704 Serial Number: 10/751,387
Location (Bldg/Room#): REM 5631 (Mailbox #): _____ Results Format Preferred (circle): PAPER DISK

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Isotopically enriched N-substituted piperazine acetic acids & methods
Inventors (please provide full names): De-g et al

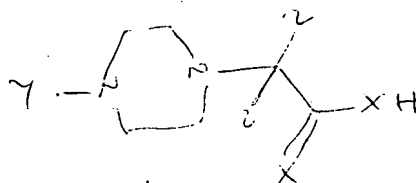
Earliest Priority Date: 01/05/04

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Compounds of formula (I) please find the various "Z" substituents on the ring and not limited to the positions on the ring



X is or is not

Y is alkyl or alkyl ether C₁-6

Z is H, deuterium, fluorine, chlorine, bromine, iodine, an amino acid

Side chain is C₁-6 alkyl optionally substituted

Thanks

STAFF USE ONLY

Searcher: Jan

Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: 5/3/07

Date Completed: 5/3/07

Searcher Prep & Review Time: 20

Online Time: 130

Type of Search

____ NA Sequence (#)

____ AA Sequence (#)

/ Structure (#)

____ Bibliographic

____ Litigation

____ Fulltext

____ Other

Vendors and cost where applicable

/ STN _____ Dialog

____ Questel/Orbit _____ Lexis/Nexis

____ Westlaw _____ WWW/Internet

____ In-house sequence systems

____ Commercial _____ Oligomer _____ Score/Length
____ Interference _____ SPDI _____ Encode/Transl

____ Other (specify)

=> fil reg

FILE 'REGISTRY' ENTERED AT 07:41:24 ON 03 MAY 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 MAY 2007 HIGHEST RN 934214-84-3

DICTIONARY FILE UPDATES: 2 MAY 2007 HIGHEST RN 934214-84-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

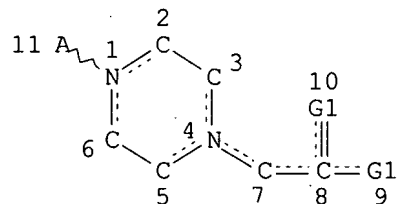
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> d sta que 127

L19 STR



VAR G1=O/S

NODE ATTRIBUTES:

NSPEC IS RC AT 11

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

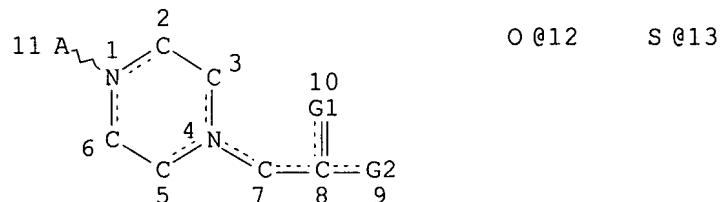
RSPEC 1

NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

L21 7570 SEA FILE=REGISTRY SSS FUL L19

L22 STR



VAR G1=O/S

VAR G2=12/13
 NODE ATTRIBUTES:
 NSPEC IS RC AT 11
 CONNECT IS E1 RC AT 12
 CONNECT IS E1 RC AT 13
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC 1
 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
 L23 SCR 2039 OR 2045 OR 2046 OR 2047
 L26 34 SEA FILE=REGISTRY SUB=L21 SSS FUL L23
 L27 17 SEA FILE=REGISTRY SUB=L26 SSS FUL L22

100.0% PROCESSED 34 ITERATIONS
 SEARCH TIME: 00.00.01

17 ANSWERS

=> d his

(FILE 'HOME' ENTERED AT 07:12:29 ON 03 MAY 2007)
 SET COST OFF

FILE 'HCAPLUS' ENTERED AT 07:12:44 ON 03 MAY 2007

L1 6 S (US20050148774 IOR US20050148771)/PN OR (US2004-751387# OR US
 E DEY/AU
 E DEY D/AU
 E DEY S/AU
 L2 559 S E3-E14
 E DEY SUB/AU
 L3 20 S E6,E7
 E SUBHAKAR/AU
 E DEY NAME/AU
 E PAPPIN/AU
 L4 113 S E9-E16
 E PURKAYASTHA/AU
 E PURKAYASTHA S/AU
 L5 35 S E3-E7,E14
 E SUBHASISH/AU
 E PILLAI/AU
 E PILLAI S/AU
 L6 304 S E3-E25,E39,E40
 E SASI/AU
 L7 5 S E17,E18
 E COULL/AU
 E COULL J/AU
 L8 144 S E3,E4,E6,E9,E10,E15
 E APPLERA/PA,CS
 L9 516 S E3-E22
 E APP BIO/PA,CS
 L10 1 S E6
 E APPL BIO/PA,CS
 L11 153 S E91-E134
 E APPLIED BIO/PA,CS
 L12 253 S E164-E252
 L13 30 S E253-E272

SEL RN L1

FILE 'REGISTRY' ENTERED AT 07:18:53 ON 03 MAY 2007

L14 138 S E1-E138
L15 73 S L14 AND NC2NC2/ES
L16 53 S L15 AND (O OR S)/ELS
L17 13 S L16 AND C7H14N2O2
L18 11 S L17 NOT (54699-92-2 OR 54699-92-2/CRN)
L19 STR
L20 50 S L19
L21 7570 S L19 FUL
SAV L21 SACKKEY751/A
L22 STR L19
L23 SCR 2039 OR 2045 OR 2046 OR 2047
L24 0 S L22 AND L23 SAM SUB=L21
L25 0 S L23 SAM SUB=L21
L26 34 S L23 FUL SUB=L21
SAV L26 SACKKEY751A/A
L27 17 S L22 FUL SUB=L26
SAV L27 SACKKEY751B/A
L28 17 S L18,L27
L29 17 S L26 NOT L28
L30 34 S L16 NOT L28,L29

FILE 'HCAPLUS' ENTERED AT 07:33:20 ON 03 MAY 2007

L31 8 S L28
L32 6 S L31 AND L1-L13
L33 1 S L31,L32 AND PY<=2004 NOT P/DT
L34 6 S L31,L32 AND (PD<=20040105 OR PRD<=20040105 OR AD<=20040105) A
L35 7 S L33,L34
L36 6 S L32 AND L35
L37 1 S L35 NOT L36
L38 1 S L31 NOT L35

FILE 'USPATFULL' ENTERED AT 07:41:09 ON 03 MAY 2007

L39 6 S L28

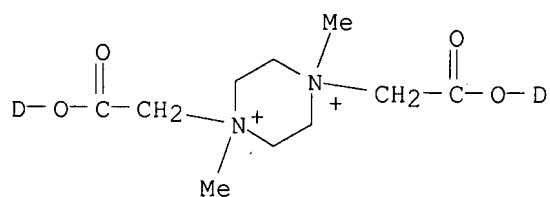
FILE 'REGISTRY' ENTERED AT 07:41:24 ON 03 MAY 2007

=> d ide can tot l27

L27 ANSWER 1 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
RN 911642-71-2 REGISTRY
ED Entered STN: 31 Oct 2006
CN Piperazinium, 1,4-bis(carboxy-d-methyl)-1,4-dimethyl-, salt with
4-hydroxybenzoic acid (1:2) (9CI) (CA INDEX NAME)
MF C10 H18 D2 N2 O4 . 2 C7 H5 O3
SR CA
LC STN Files: CA, CAPLUS

CM 1

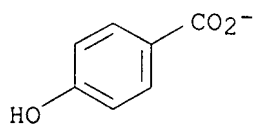
CRN 911642-70-1
CMF C10 H18 D2 N2 O4



CM 2

CRN 456-23-5

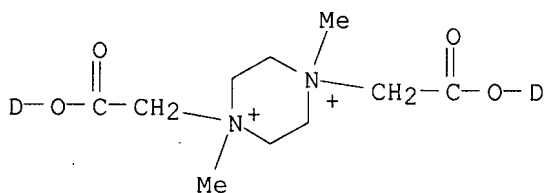
CMF C7 H5 O3



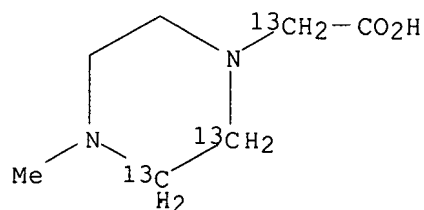
1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 145:396865

L27 ANSWER 2 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 911642-70-1 REGISTRY
 ED Entered STN: 31 Oct 2006
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 CI COM
 SR CA



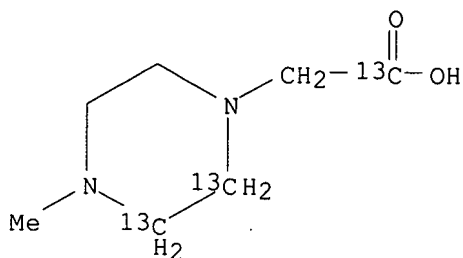
L27 ANSWER 3 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 857291-38-4 REGISTRY
 ED Entered STN: 27 Jul 2005
 CN 1-Piperazine-2,3-13C2-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)
 MF C7 H14 N2 O2
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:112150

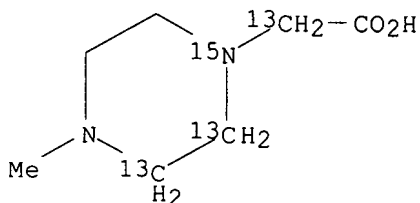
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RN 857291-36-2 REGISTRY
ED Entered STN: 27 Jul 2005
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MF C7 H14 N2 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:112150

L27 ANSWER 5 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
RN 857027-12-4 REGISTRY
ED Entered STN: 26 Jul 2005
CN 1-Piperazine-2,3-13C2-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)
MF C7 H14 N2 O2
SR CA
LC STN Files: CA, CAPLUS, MSDS-OHS, USPATFULL



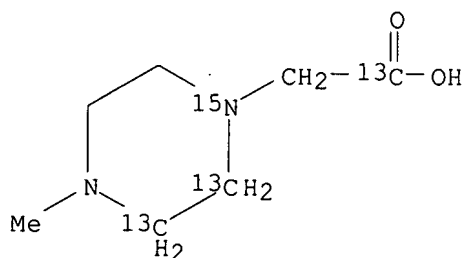
3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:115568

REFERENCE 2: 143:93642

REFERENCE 3: 143:93635

L27 ANSWER 6 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
RN 857027-11-3 REGISTRY
ED Entered STN: 26 Jul 2005
CN 1-Piperazine-2,3-¹³C2-1-¹⁵N-acetic-carboxy-¹³C acid, 4-methyl- (9CI) (CA
INDEX NAME)
MF C7 H14 N2 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



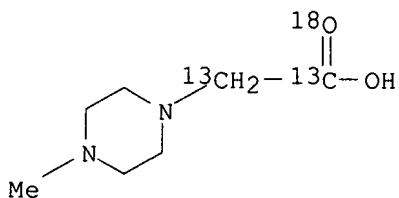
3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:115568

REFERENCE 2: 143:93642

REFERENCE 3: 143:93635

L27 ANSWER 7 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
RN 857027-06-6 REGISTRY
ED Entered STN: 26 Jul 2005
CN 1-Piperazineacetic-carboxy, α -¹³C2-¹⁸O acid, 4-methyl- (9CI) (CA
INDEX NAME)
MF C7 H14 N2 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



3 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

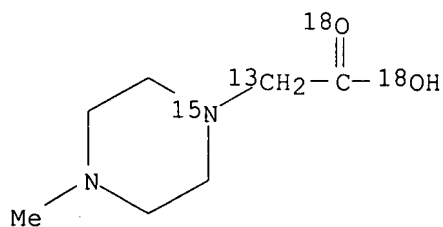
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:112150

REFERENCE 2: 143:93642

REFERENCE 3: 143:93635

L27 ANSWER 8 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
RN 856290-55-6 REGISTRY
ED Entered STN: 21 Jul 2005
CN 1-Piperazineacetic- α -¹³C-1-¹⁵N-¹⁸O₂ acid, 4-methyl- (9CI) (CA INDEX
NAME)
MF C7 H14 N2 O2
CI COM
SR CA
LC STN Files: CA, CAPLUS, MSDS-OHS, USPATFULL



4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

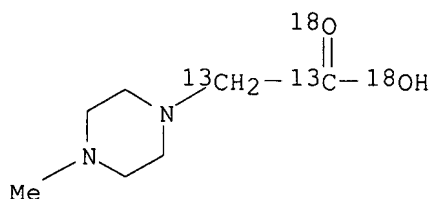
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REFERENCE 2: 143:112150

REFERENCE 3: 143:93642

REFERENCE 4: 143:93635

L27 ANSWER 9 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
RN 856290-53-4 REGISTRY
ED Entered STN: 21 Jul 2005
CN 1-Piperazineacetic-carboxy, α -¹³C₂-¹⁸O₂ acid, 4-methyl- (9CI) (CA
INDEX NAME)
MF C7 H14 N2 O2
CI COM
SR CA
LC STN Files: CA, CAPLUS, MSDS-OHS, USPATFULL



4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

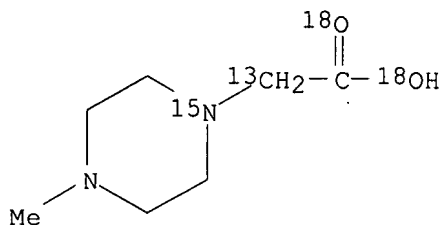
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REFERENCE 2: 143:112150

REFERENCE 3: 143:93642

REFERENCE 4: 143:93635

L27 ANSWER 10 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
RN 856188-13-1 REGISTRY
ED Entered STN: 20 Jul 2005
CN 1-Piperazineacetic- α -¹³C-1-¹⁵N-18O₂ acid, 4-methyl-, dihydrochloride
(9CI) (CA INDEX NAME)
MF C7 H14 N2 O2 . 2 Cl H
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
CRN (856290-55-6)



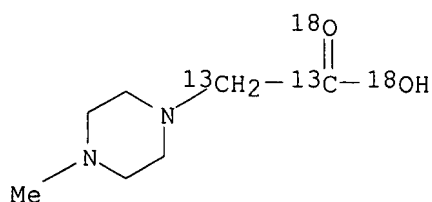
● 2 HCl

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:97398

REFERENCE 2: 143:93642

L27 ANSWER 11 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
RN 856187-92-3 REGISTRY
ED Entered STN: 20 Jul 2005
CN 1-Piperazineacetic-carboxy, α -¹³C₂-18O₂ acid, 4-methyl-,
dihydrochloride (9CI) (CA INDEX NAME)
MF C7 H14 N2 O2 . 2 Cl H
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
CRN (856290-53-4)



● 2 HCl

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

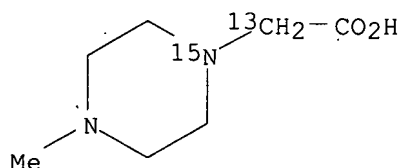
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REFERENCE 3: 143:97398

REFERENCE 4: 143:93642

L27 ANSWER 12 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
RN 856187-76-3 REGISTRY
ED Entered STN: 20 Jul 2005
CN 1-Piperazine-1-15N-acetic- α -13C acid, 4-methyl- (9CI) (CA INDEX
NAME)
MF C7 H14 N2 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:115574

REFERENCE 2: 143:115568

REFERENCE 3: 143:112150

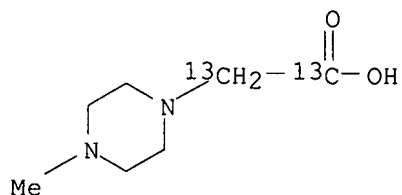
REFERENCE 4: 143:97398

REFERENCE 5: 143:93642

REFERENCE 6: 143:93635

L27 ANSWER 13 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
RN 856187-68-3 REGISTRY

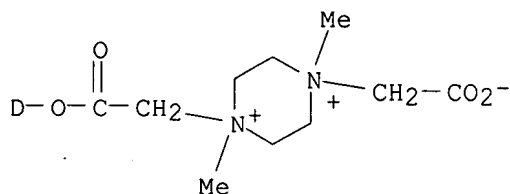
ED Entered STN: 20 Jul 2005
 CN 1-Piperazineacetic-carboxy, α -¹³C2 acid, 4-methyl- (9CI) (CA INDEX NAME)
 MF C7 H14 N2 O2
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



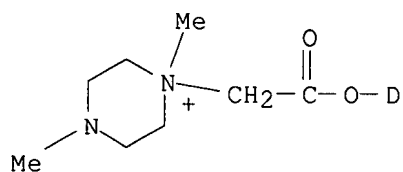
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 6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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 REFERENCE 3: 143:112150
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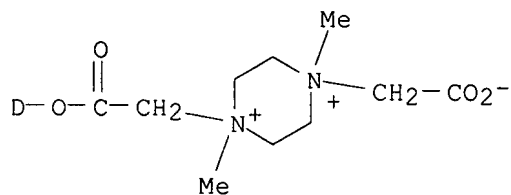
L27 ANSWER 14 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 752198-16-6 REGISTRY
 ED Entered STN: 27 Sep 2004
 CN Piperazinium, 1-(carboxymethyl)-4-(carboxy-d-methyl)-1,4-dimethyl-, mono(inner salt) (9CI) (CA INDEX NAME)
 MF C10 H18 D N2 O4
 CI COM
 SR CA



L27 ANSWER 15 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 748128-11-2 REGISTRY
 ED Entered STN: 20 Sep 2004
 CN Piperazinium, 1-(carboxy-d-methyl)-1,4-dimethyl- (9CI) (CA INDEX NAME)
 MF C8 H16 D N2 O2
 CI COM
 SR CA



L27 ANSWER 16 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 488721-94-4 REGISTRY
 ED Entered STN: 11 Feb 2003
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 LC STN Files: CA, CAPLUS
 CRN (752198-16-6)

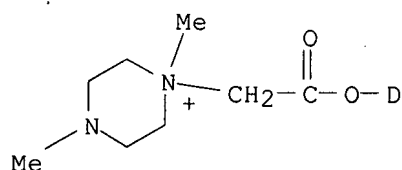


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1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:122357

L27 ANSWER 17 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 488721-93-3 REGISTRY
 ED Entered STN: 11 Feb 2003
 CN Piperazinium, 1-(carboxy-d-methyl)-1,4-dimethyl-, chloride, hydrochloride-d (9CI) (CA INDEX NAME)
 MF C8 H16 D N2 O2 . Cl D . Cl
 SR CA
 LC STN Files: CA, CAPLUS
 CRN (748128-11-2)



● Cl⁻

● DCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:122357

=> fil uspatful

FILE 'USPATFULL' ENTERED AT 07:41:44 ON 03 MAY 2007

CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 1 May 2007 (20070501/PD)

FILE LAST UPDATED: 1 May 2007 (20070501/ED)

HIGHEST GRANTED PATENT NUMBER: US7213269

HIGHEST APPLICATION PUBLICATION NUMBER: US2007094759

CA INDEXING IS CURRENT THROUGH 1 May 2007 (20070501/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 1 May 2007 (20070501/PD)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2006

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2006

=> d bib abs hitstr tot 139

L39 ANSWER 1 OF 6 USPATFULL on STN

AN 2005:172025 USPATFULL

TI Isotopically enriched N-substituted piperazine acetic acids and methods
for the preparation thereof

IN Dey, Subhakar, Billerica, MA, UNITED STATES
Pappin, Darryl J.C., Boxborough, MA, UNITED STATES
Purkayastha, Subhasish, Acton, MA, UNITED STATES
Pillai, Sasi, Littleton, MA, UNITED STATES
Coull, James M., Westford, MA, UNITED STATES

PA Applera Corporation. (U.S. corporation)

PI US 2005148774 A1 20050707

AI US 2004-751387 A1 20040105 (10)

DT Utility

FS APPLICATION

LREP APPLIED BIOSYSTEMS, 500 OLD CONNECTICUT PATH, FRAMINGHAM, MA, 01701, US

CLMN Number of Claims: 22

ECL Exemplary Claim: 1

DRWN 11 Drawing Page(s)

LN.CNT 1451

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB In some embodiments, this invention pertains to isotopically enriched N-substituted piperazine acetic acids. In some embodiments, this invention pertains to methods for the preparation of isotopically enriched N-substituted piperazine acetic acids.

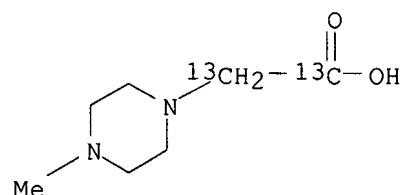
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **856187-68-3P**

(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

RN 856187-68-3 USPATFULL

CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ acid, 4-methyl- (9CI) (CA INDEX NAME)



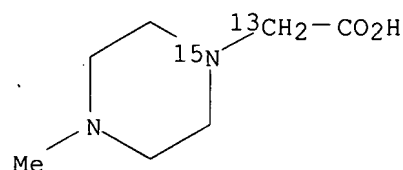
IT **856187-76-3P 856187-92-3P 856290-53-4P**

856290-55-6P 857027-11-3P 857027-12-4P

(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

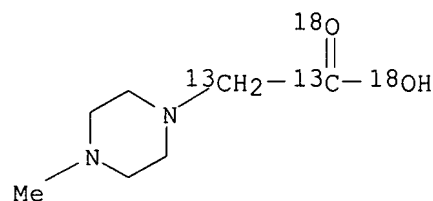
RN 856187-76-3 USPATFULL

CN 1-Piperazine-1- ^{15}N -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856187-92-3 USPATFULL

CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ - $^{18}\text{O}_2$ acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

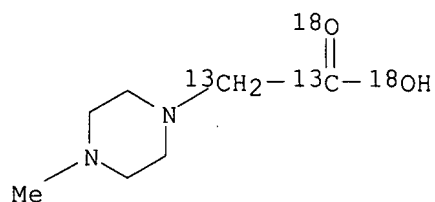


● 2 HCl

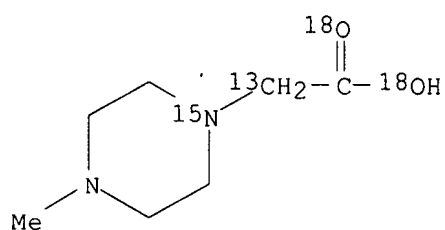
RN 856290-53-4 USPATFULL

CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ - $^{18}\text{O}_2$ acid, 4-methyl- (9CI) (CA

INDEX NAME)

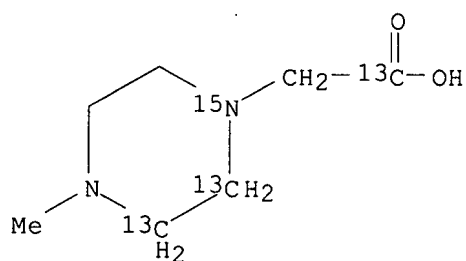


RN 856290-55-6 USPATFULL

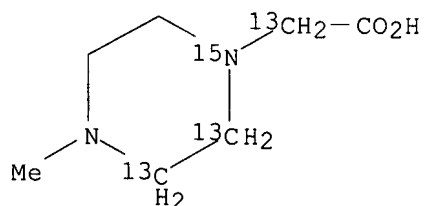
CN 1-Piperazineacetic- α -13C-1-15N-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)

RN 857027-11-3 USPATFULL

CN 1-Piperazine-2,3-13C2-1-15N-acetic-carboxy-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-12-4 USPATFULL

CN 1-Piperazine-2,3-13C2-1-15N-acetic- α -13C acid, 4-methyl- (9CI) (CA INDEX NAME)

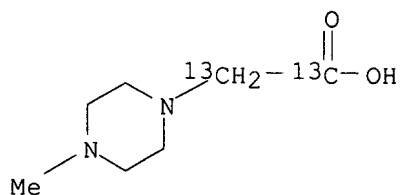
L39 ANSWER 2 OF 6 USPATFULL on STN

AN 2005:172024 USPATFULL

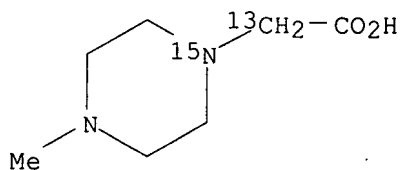
TI Isotopically enriched N-substituted piperazines and methods for the preparation thereof
 IN Pappin, Darryl J.C., Boxborough, MA, UNITED STATES
 Pillai, Sasi, Littleton, MA, UNITED STATES
 Coull, James M., Westford, MA, UNITED STATES
 PA Applera Corporation. (U.S. corporation)
 PI US 2005148773 A1 20050707
 AI US 2004-751388 A1 20040105 (10)
 DT Utility
 FS APPLICATION
 LREP APPLIED BIOSYSTEMS, 500 OLD CONNECTICUT PATH, FRAMINGHAM, MA, 01701, US
 CLMN Number of Claims: 17
 ECL Exemplary Claim: 1
 DRWN 11 Drawing Page(s)
 LN.CNT 1418
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.
 AB In some embodiments, this invention pertains to isotopically enriched N-substituted piperazines. In some embodiments, this invention pertains to methods for the preparation of isotopically enriched N-substituted piperazines.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

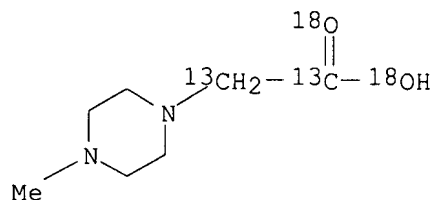
IT **856187-68-3P**
 (preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)
 RN 856187-68-3 USPATFULL
 CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ acid, 4-methyl- (9CI) (CA INDEX NAME)



IT **856187-76-3P 856187-92-3P**
 (preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)
 RN 856187-76-3 USPATFULL
 CN 1-Piperazine-1- ^{15}N -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)

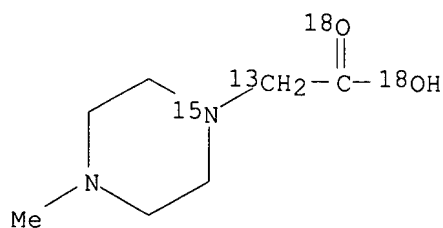


RN 856187-92-3 USPATFULL
 CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ - $^{18}\text{O}_2$ acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

L39 ANSWER 3 OF 6 USPATFULL on STN
 AN 2005:172022 USPATFULL
 TI Active esters of N-substituted piperazine acetic acids, including isotopically enriched versions thereof
 IN Dey, Subhakar, Billerica, MA, UNITED STATES
 Pappin, Darryl J.C., Boxborough, MA, UNITED STATES
 Purkayastha, Subhasish, Acton, MA, UNITED STATES
 Pillai, Sasi, Littleton, MA, UNITED STATES
 Coull, James M., Westford, MA, UNITED STATES
 PA Applera Corporation. (U.S. corporation)
 PI US 2005148771 A1 20050707
 AI US 2004-751354 A1 20040105 (10)
 DT Utility
 FS APPLICATION
 LREP APPLIED BIOSYSTEMS, 500 OLD CONNECTICUT PATH, FRAMINGHAM, MA, 01701, US
 CLMN Number of Claims: 49
 ECL Exemplary Claim: 1
 DRWN 11 Drawing Page(s)
 LN.CNT 1557
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.
 AB In some embodiments, this invention pertains to active esters of N-substituted piperazine acetic acid, including isotopically enriched versions thereof. In some embodiments, this invention pertains to methods for the preparation of active esters of N-substituted piperazine acetic acid, including isotopically enriched versions thereof.
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.
 IT **856188-13-1**
 (preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)
 RN 856188-13-1 USPATFULL
 CN 1-Piperazineacetic- α -13C-1-15N-18O2 acid, 4-methyl-, dihydrochloride
 (9CI) (CA INDEX NAME)



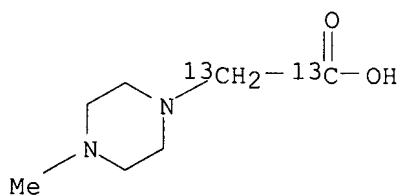
●2 HCl

IT 856187-68-3P

(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

RN 856187-68-3 USPATFULL

CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ acid, 4-methyl- (9CI) (CA INDEX NAME)

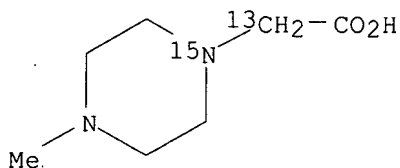


IT 856187-76-3P 856187-92-3P

(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

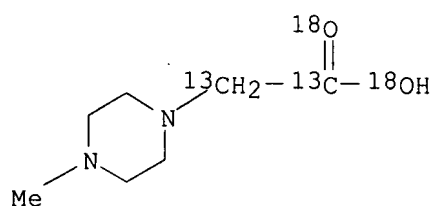
RN 856187-76-3 USPATFULL

CN 1-Piperazine-1- ^{15}N -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856187-92-3 USPATFULL

CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ - $^{18}\text{O}_2$ acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

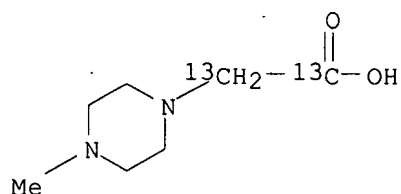


● 2 HCl

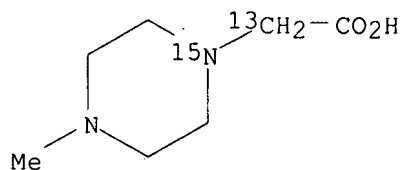
L39 ANSWER 4 OF 6 USPATFULL on STN
 AN 2005:171340 USPATFULL
 TI Isobarically labeled analytes and fragment ions derived therefrom
 IN Pappin, Darryl J.C., Boxborough, MA, UNITED STATES
 Purkayastha, Subhasish, Acton, MA, UNITED STATES
 Coull, James M., Westford, MA, UNITED STATES
 PA Applera Corporation (U.S. corporation)
 PI US 2005148087 A1 20050707
 AI US 2004-852730 A1 20040524 (10)
 RLI Continuation-in-part of Ser. No. US 2004-822639, filed on 12 Apr 2004,
 PENDING Continuation-in-part of Ser. No. US 2004-751353, filed on 5 Jan
 2004, PENDING
 DT Utility
 FS APPLICATION
 LREP APPLIED BIOSYSTEMS, 500 OLD CONNECTICUT PATH, FRAMINGHAM, MA, 01701, US
 CLMN Number of Claims: 18
 ECL Exemplary Claim: 1
 DRWN 35 Drawing Page(s)
 LN.CNT 4527
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.
 AB This invention pertains to isobarically labeled analytes and fragment
 ions thereof.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 856187-68-3P 856187-76-3P 856290-53-4P
 856290-55-6P 857027-06-6P 857291-36-2P
 857291-38-4P
 (isobarically labeled analytes and fragment ions derived therefrom)
 RN 856187-68-3 USPATFULL
 CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ acid, 4-methyl- (9CI) (CA INDEX
 NAME)

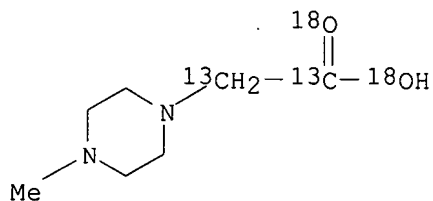


RN 856187-76-3 USPATFULL
 CN 1-Piperazine-1- ^{15}N -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX
 NAME)



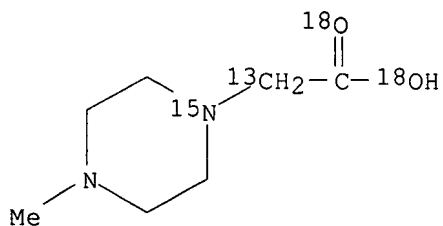
RN 856290-53-4 USPATFULL

CN 1-Piperazineacetic-carboxy, α - ^{13}C - ^{18}O acid, 4-methyl- (9CI) (CA INDEX NAME)



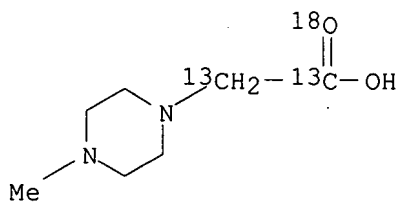
RN 856290-55-6 USPATFULL

CN 1-Piperazineacetic- α - ^{13}C -1- ^{15}N - ^{18}O acid, 4-methyl- (9CI) (CA INDEX NAME)



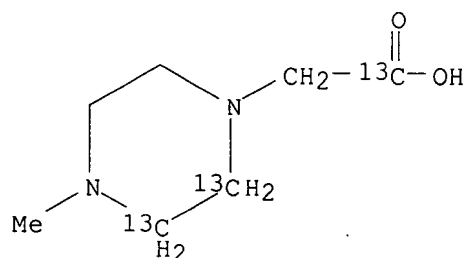
RN 857027-06-6 USPATFULL

CN 1-Piperazineacetic-carboxy, α - ^{13}C - ^{18}O acid, 4-methyl- (9CI) (CA INDEX NAME)



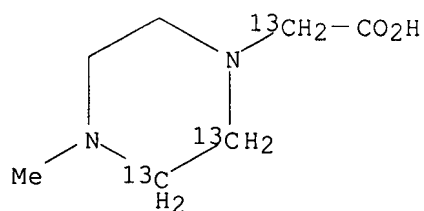
RN 857291-36-2 USPATFULL

CN 1-Piperazine-2,3- ^{13}C -acetic-carboxy- ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857291-38-4 USPATFULL

CN 1-Piperazine-2,3-13C2-acetic- α -13C acid, 4-methyl- (9CI) (CA INDEX NAME)



L39 ANSWER 5 OF 6 USPATFULL on STN

AN 2005:171238 USPATFULL

TI Mixtures of isobarically labeled analytes and fragments ions derived therefrom

IN Pappin, Darryl J. C., Boxborough, MA, UNITED STATES

Purkayastha, Subhasish, Acton, MA, UNITED STATES

Coull, James M., Westford, MA, UNITED STATES

PA Applera Corporation (U.S. corporation)

PI US 2005147985 A1 20050707

AI US 2004-822639 A1 20040412 (10)

RLI Continuation-in-part of Ser. No. US 2004-751353, filed on 5 Jan 2004, PENDING

DT Utility

FS APPLICATION

LREP APPLIED BIOSYSTEMS, 500 OLD CONNECTICUT PATH, FRAMINGHAM, MA, 01701, US

CLMN Number of Claims: 13

ECL Exemplary Claim: 1

DRWN 13 Drawing Page(s)

LN.CNT 1939

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention pertains to mixtures of isobarically labeled analytes and fragment ions thereof.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

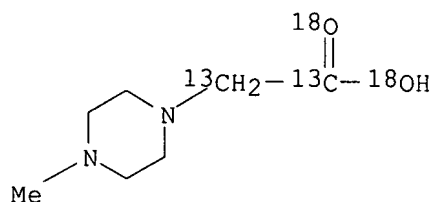
IT 856290-53-4P 856290-55-6P 857027-11-3P

857027-12-4P

(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

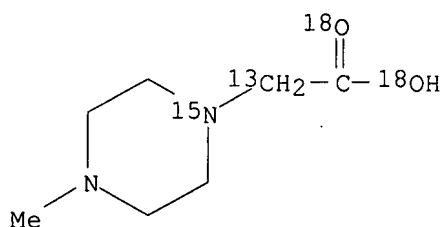
RN 856290-53-4 USPATFULL

CN 1-Piperazineacetic-carboxy, α -13C2-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



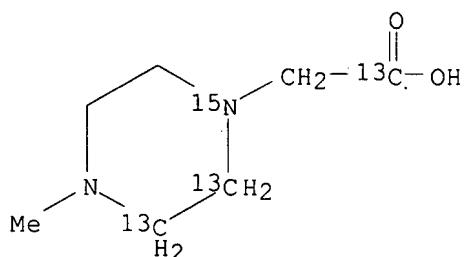
RN 856290-55-6 USPATFULL

CN 1-Piperazineacetic- α - ^{13}C -1- ^{15}N - $^{18}\text{O}_2$ acid, 4-methyl- (9CI) (CA INDEX NAME)



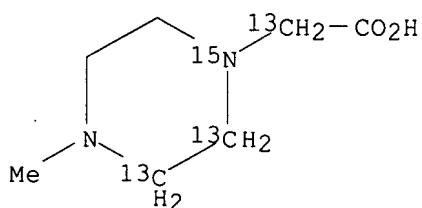
RN 857027-11-3 USPATFULL

CN 1-Piperazine-2,3- $^{13}\text{C}_2$ -1- ^{15}N -acetic-carboxy- ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-12-4 USPATFULL

CN 1-Piperazine-2,3- $^{13}\text{C}_2$ -1- ^{15}N -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)

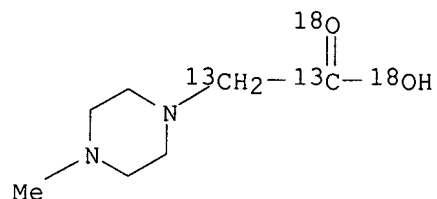


IT 856187-92-3 856188-13-1

(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

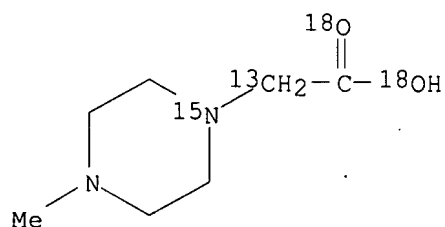
RN 856187-92-3 USPATFULL

CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ - $^{18}\text{O}_2$ acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



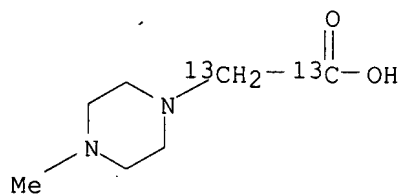
● 2 HCl

RN 856188-13-1 USPATFULL
 CN 1-Piperazineacetic- α - ^{13}C - ^{15}N - $^{18}\text{O}_2$ acid, 4-methyl-, dihydrochloride
 (9CI) (CA INDEX NAME)

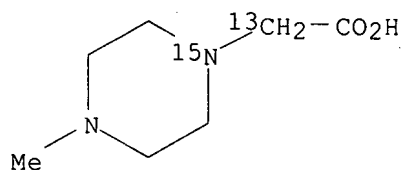


● 2 HCl

IT 856187-68-3P
 (mixts. of isobarically labeled analytes and fragments ions derived
 therefrom)
 RN 856187-68-3 USPATFULL
 CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ acid, 4-methyl- (9CI) (CA INDEX
 NAME)

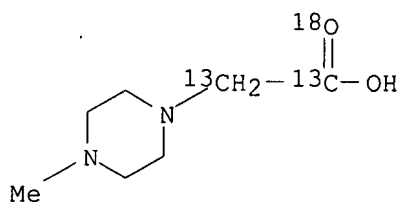


IT 856187-76-3P 857027-06-6DP, salts
 (mixts. of isobarically labeled analytes and fragments ions derived
 therefrom)
 RN 856187-76-3 USPATFULL
 CN 1-Piperazine- ^{15}N -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX
 NAME)



RN 857027-06-6 USPATFULL

CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ - ^{18}O acid, 4-methyl- (9CI) (CA INDEX NAME)



L39 ANSWER 6 OF 6 USPATFULL on STN

AN 2005:171235 USPATFULL

TI Mixtures of isobarically labeled analytes and fragments ions derived therefrom

IN Pappin, Darryl J.C., Boxborough, MA, UNITED STATES

Purkayastha, Subhasish, Acton, MA, UNITED STATES

Coull, James M., Westford, MA, UNITED STATES

PA Applera Corporation (U.S. corporation)

PI US 2005147982 A1 20050707

AI US 2004-751353 A1 20040105 (10)

DT Utility

FS APPLICATION

LREP APPLIED BIOSYSTEMS, 500 OLD CONNECTICUT PATH, FRAMINGHAM, MA, 01701, US

CLMN Number of Claims: 13

ECL Exemplary Claim: 1

DRWN 11 Drawing Page(s)

LN.CNT 1379

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention pertains to mixtures of isobarically labeled analytes and fragment ions thereof.

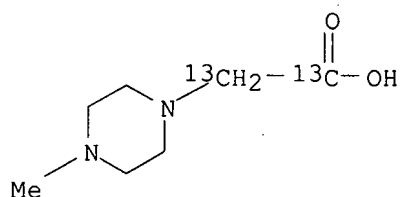
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **856187-68-3P**

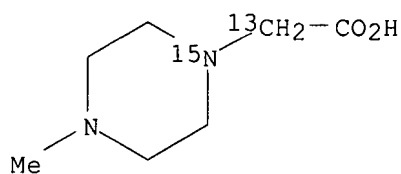
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

RN 856187-68-3 USPATFULL

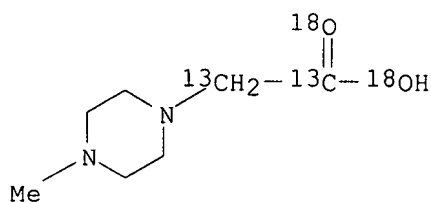
CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ acid, 4-methyl- (9CI) (CA INDEX NAME)



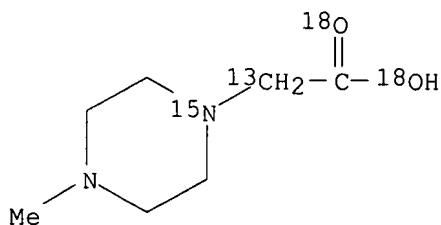
IT 856187-76-3P 856290-53-4P 856290-55-6P
 857027-06-6DP, salts 857027-11-3P 857027-12-4P
 (mixts. of isobarically labeled analytes and fragments ions derived
 therefrom)
 RN 856187-76-3 USPATFULL
 CN 1-Piperazine-1-15N-acetic- α -13C acid, 4-methyl- (9CI) (CA INDEX
 NAME)



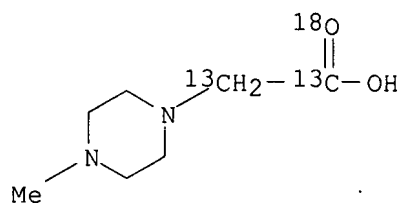
RN 856290-53-4 USPATFULL
 CN 1-Piperazineacetic-carboxy, α -13C2-18O2 acid, 4-methyl- (9CI) (CA
 INDEX NAME)



RN 856290-55-6 USPATFULL
 CN 1-Piperazineacetic- α -13C-1-15N-18O2 acid, 4-methyl- (9CI) (CA INDEX
 NAME)

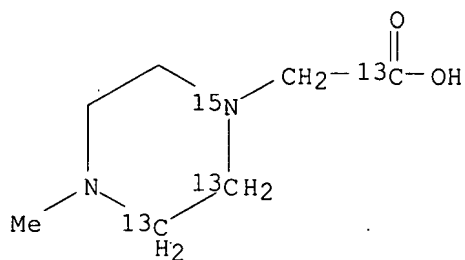


RN 857027-06-6 USPATFULL
 CN 1-Piperazineacetic-carboxy, α -13C2-18O acid, 4-methyl- (9CI) (CA
 INDEX NAME)



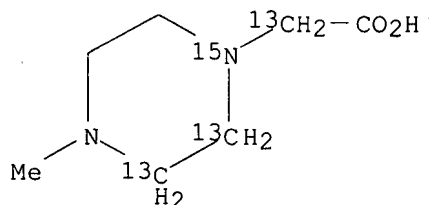
RN 857027-11-3 USPATFULL

CN 1-Piperazine-2,3-13C2-1-15N-acetic-carboxy-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-12-4 USPATFULL

CN 1-Piperazine-2,3-13C2-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



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FILE COVERS 1907 - 3 May 2007 VOL ISS

FILE LAST UPDATED: 2 May 2007 (20070502/ED)

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FILE COVERS 1907 - 3 May 2007 VOL 146 ISS 19

jan delaval - 3 may 2007

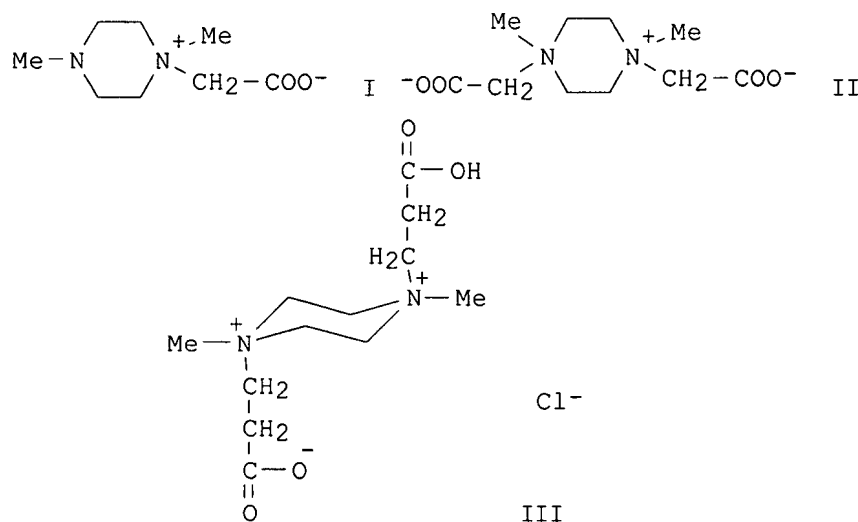
FILE LAST UPDATED: 1 May 2007 (20070501/ED)

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L37 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
 AN 2002:675170 HCAPLUS
 DN 138:122357
 TI Molecular structure, hydrogen bonding, basicity and spectroscopic
 properties of N,N'-dimethylpiperazine betaines and their hydrohalides
 AU Dega-Szafran, Z.; Jaskolski, M.; Kurzyca, I.; Barczynski, P.; Szafran, M.
 CS Faculty of Chemistry, Adam Mickiewicz University, Poznan, 60-780, Pol.
 SO Journal of Molecular Structure (2002), 614(1-3), 23-32
 CODEN: JMOSB4; ISSN: 0022-2860
 PB Elsevier Science B.V.
 DT Journal
 LA English
 GI



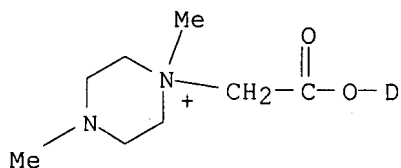
AB Two N,N'-dimethylpiperazine betaines [mono (I) and double (II)] have been synthesized. Betaine I reacts with two equivalent of HCl or HBr, while II only with one. In the crystal structure of N,N'-dicarboxymethyl-N,N'-dimethylpiperazine monohydrochloride (N,N'-dimethylpiperazine doublebetaine monohydrochloride, III) determined by X-ray diffraction, the piperazinium moieties form infinite chains bridged by very strong, sym. and linear hydrogen bonds (O...O 2.460(2) Å). The piperazine ring adopts a chair conformation with the CH₂COOH group in the axial and the Me group in the equatorial positions. The N⁺ atoms interact electrostatically with the Cl⁻ ion and the oxygen atoms of the carboxylate groups. The FTIR spectrum of 7-Cl shows an intense broad absorption in the 1500-400 cm⁻¹ region and a νC:O band at 1734 cm⁻¹. The pK_a values of I and II were determined by potentiometric titration. The ¹H and ¹³C NMR spectra in D₂O were analyzed.

IT 488721-93-3P 488721-94-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, mol. structure, hydrogen bonding, basicity and spectroscopic
 properties of N,N'-dimethylpiperazine betaines and their hydrohalides)

RN 488721-93-3 HCAPLUS

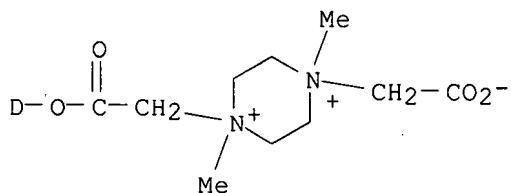
CN Piperazinium, 1-(carboxy-d-methyl)-1,4-dimethyl-, chloride,
 hydrochloride-d (9CI) (CA INDEX NAME)

● Cl⁻

● DCl

RN 488721-94-4 HCAPLUS

CN Piperazinium, 1,4-bis(carboxy-d-methyl)-1,4-dimethyl-, inner salt,
 chloride (9CI) (CA INDEX NAME)

● Cl⁻

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Albert, A	1962			Ionization Constants	
Allinger, N	1965	87	1232	J Am Chem Soc	HCAPLUS
Baltzly, R	1954	76	1164	J Am Chem Soc	HCAPLUS
Baltzly, R	1954	76	1165	J Am Chem Soc	HCAPLUS
Baltzly, R	1955	77	14809	J Am Chem Soc	HCAPLUS
Barczynski, P	1998	72	277	Pol J Chem	HCAPLUS
Barczynski, P	2000	74	1149	Pol J Chem	HCAPLUS
Coddington, J	1990	46A	1487	Spectrochim Acta	HCAPLUS
Dega-Szafran, Z	1993		316	J Chem Res Synop	HCAPLUS
Dega-Szafran, Z	1998		296	J Chem Res Synop	HCAPLUS
Dega-Szafran, Z	1994	322	297	J Mol Struct	HCAPLUS
Dega-Szafran, Z	1997	436-4	107	J Mol Struct	HCAPLUS

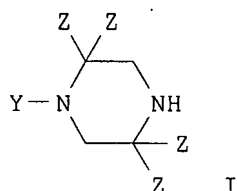
Dega-Szafran, Z	1999	478	49	J Mol Struct	HCAPLUS
Dega-Szafran, Z	2000	555	67	J Mol Struct	HCAPLUS
Dega-Szafran, Z	2002	605	309	J Mol Struct	HCAPLUS
Dega-Szafran, Z	2002	605	325	J Mol Struct	HCAPLUS
Dega-Szafran, Z	2000	38	43	Magn Reson Chem	HCAPLUS
Eicher, T	1995		422	The Chemistry of Het	
Eliel, E	1994			Stereochemistry of O	
Harfenist, M	1957	79	2211	J Am Chem Soc	HCAPLUS
Kuma Diffraction	1999	162		CrysAlis	
Lowik, D	2000	41	1837	Tetrahedron Lett	HCAPLUS
McConnaughie, A	1994	37	1063	J Med Chem	HCAPLUS
Moore, T	1929		39	J Chem Soc	HCAPLUS
Oesch, U	1986	58	2285	Anal Chem	HCAPLUS
Ram, S	1985	26	5367	Tetrahedron Lett	HCAPLUS
Schwarzenbach, G	1952	35	2333	Helv Chim Acta	HCAPLUS
Sheldrick, G	1997			SHELXL97, Program fo	
Sheldrick, G	1997			SHELXL97, Program fo	
Smith, D	1950	72	2969	J Am Chem Soc	HCAPLUS
Smith, D	1951	73	2964	J Am Chem Soc	HCAPLUS
Suzuki, T	1997	40	2047	J Med Chem	HCAPLUS
Szafran, M	1999	39	253	Isr J Chem	HCAPLUS
Szafran, M	2001	598	251	J Mol Struct	HCAPLUS
Szafran, M	2001	598	265	J Mol Struct	
Szafran, M	2001	563-5	555	J Mol Struct	HCAPLUS
Szafran, M	2000	23	1	Vib Spectrosc	HCAPLUS
Taylor, M	1988	26	619	Magn Reson Chem	HCAPLUS
Ziegler, E	1985	116	821	Monatsh Chem	HCAPLUS

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L36 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
 AN 2005:592130 HCAPLUS
 DN 143:115574
 TI Preparation of isotopically enriched N-substituted piperazines
 IN Pappin, Darryl J. C.; Pillai, Sasi; Coull, James .
 M.
 PA Applera Corp., USA
 SO U.S. Pat. Appl. Publ., 29 pp.
 CODEN: USXXCO
 DT Patent
 LA English
 FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 2005148773	A1	20050707	US 2004-751388	20040105	<--
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	CA 2552304	A1	20050728	CA 2005-2552304	20050105	<--
	WO 2005068446	A1	20050728	WO 2005-US223	20050105	<--
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	GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,					
	LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,					
	NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,					
	TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
	RW:					
	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,					
	AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,					
	EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,					
	RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,					
	MR, NE, SN, TD, TG					

EP 1701945 A1 20060920 EP 2005-705033 20050105 <--
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 IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS
 PRAI US 2004-751353 A 20040105 <--
 US 2004-751354 A 20040105 <--
 US 2004-751387 A 20040105 <--
 US 2004-751388 A 20040105 <--
 US 2004-822639 A 20040412
 US 2004-852730 A 20040524
 WO 2005-US223 W 20050105 <--
 OS MARPAT 143:115574
 GI

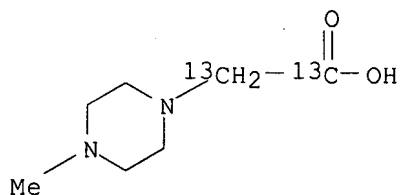


- AB Isotopically enriched N-substituted piperazines (I) or salts thereof, comprising one or more heavy atom isotopes (Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or fluorine atoms; Z = independently H, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H or F atoms, a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms), or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group; wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms; wherein the N-methylpiperazine is isotopically enriched with either of ¹³C and/or ¹⁵N) are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like (no data). Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-¹³C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-¹³C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-¹³C.
- IT **856187-68-3P 856187-92-3P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

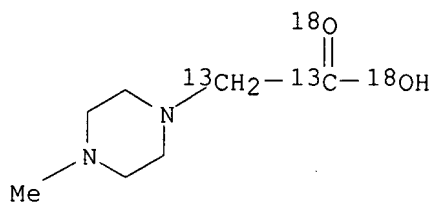
RN 856187-68-3 HCAPLUS

CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856187-92-3 HCAPLUS

CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ - $^{18}\text{O}_2$ acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



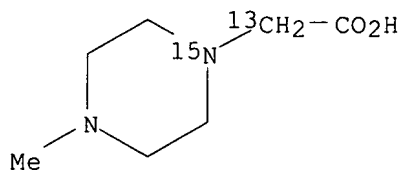
● 2 HCl

IT 856187-76-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

RN 856187-76-3 HCAPLUS

CN 1-Piperazine-1- ^{15}N -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)



L36 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:592129 HCAPLUS

DN 143:97398

TI Preparation of active esters of N-substituted piperazine acetic acids, including isotopically enriched versions

IN Dey, Subhakar; Pappin, Darryl J. C.; Purkayastha, Subhasish; Pillai, Sasi; Coull, James M.

PA Applera Corp., USA

SO U.S. Pat. Appl. Publ., 33 pp.

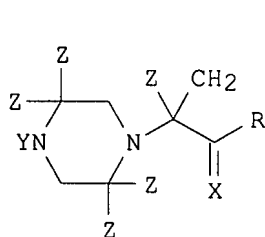
CODEN: USXXCO

DT Patent

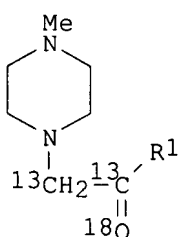
LA English

FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005148771	A1	20050707	US 2004-751354	20040105 <--
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	CA 2552304	A1	20050728	CA 2005-2552304	20050105 <--
	WO 2005068446	A1	20050728	WO 2005-US223	20050105 <--
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	EP 1701945	A1	20060920	EP 2005-705033	20050105 <--
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PRAI	US 2004-751353	A	20040105	<--	
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	US 2004-751388	A	20040105	<--	
	US 2004-822639	A	20040412		
	US 2004-852730	A	20040524		
	WO 2005-US223	W	20050105	<--	
OS	MARPAT 143:97398				
GI					



I



II

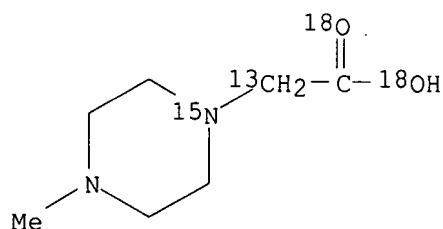
AB In some embodiments, this invention pertains to active esters of N-substituted piperazine acetic acid I (R = leaving group; X = O, S; Y = C1-C6 alkyl, C1-C6 alkyl ether; Z = H, 2H, F, Cl, Br, iodide, amino acid side chain, C1-C6 alkyl, C1-C6 alkyl ether), including isotopically enriched versions thereof. In some embodiments, this invention pertains to methods for the preparation of active esters of N-substituted piperazine acetic acid, including isotopically enriched versions thereof. For example, the isotopically labeled N-methylpiperazine II (R1 = 18OH) reacted with the trifluoroacetic acid ester of N-hydroxysuccinimide to give the succinate II (R1 = OR2, R2 = succinimido).

IT 856188-13-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

RN 856188-13-1 HCAPLUS

CN 1-Piperazineacetic- α - ^{13}C -1- ^{15}N -1802 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

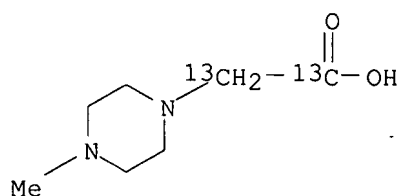
IT 856187-68-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

RN 856187-68-3 HCAPLUS

CN 1-Piperazineacetic-carboxy, α - ^{13}C 2 acid, 4-methyl- (9CI) (CA INDEX NAME)



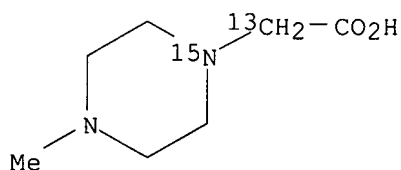
IT 856187-76-3P 856187-92-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

RN 856187-76-3 HCAPLUS

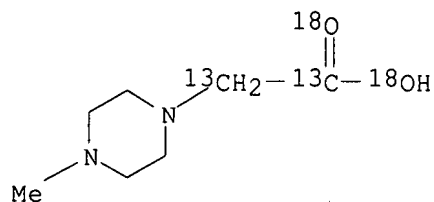
CN 1-Piperazine-1- ^{15}N -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856187-92-3 HCAPLUS

CN 1-Piperazineacetic-carboxy, α - ^{13}C 2-1802 acid, 4-methyl-,

dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

L36 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
 AN 2005:592027 HCAPLUS
 DN 143:93642
 TI Mixtures of isobarically labeled analytes and fragments ions derived therefrom
 IN Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.
 PA Applera Corp., USA
 SO U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S. Ser. No. 751,353. CODEN: USXXCO
 DT Patent
 LA English
 FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005147985	A1	20050707	US 2004-822639	20040412 <--
	US 2005147982	A1	20050707	US 2004-751353	20040105 <--
	US 2005148087	A1	20050707	US 2004-852730	20040524 <--
	AU 2005205522	A1	20050728	AU 2005-205522	20050105 <--
	CA 2552304	A1	20050728	CA 2005-2552304	20050105 <--
	WO 2005068446	A1	20050728	WO 2005-US223	20050105 <--
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	RW:			BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	
EP	1701945	A1	20060920	EP 2005-705033	20050105 <--
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PRAI	US 2004-751353	A2	20040105	<--	
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	US 2004-751388	A	20040105	<--	
	US 2004-822639	A2	20040412		
	US 2004-852730	A	20040524		
	WO 2005-US223	W	20050105	<--	
OS	MARPAT 143:93642				

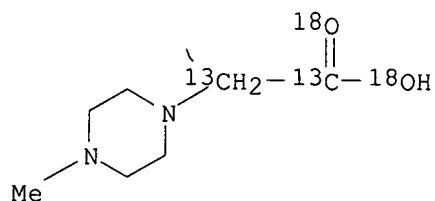
AB This invention pertains to mixts. of isobarically labeled analytes and fragment ions thereof.

IT **856290-53-4P 856290-55-6P 857027-11-3P 857027-12-4P**

RL: FMU (Formation, unclassified); SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

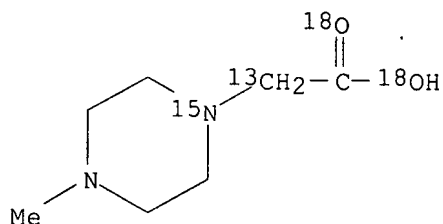
RN 856290-53-4 HCAPLUS

CN 1-Piperazineacetic-carboxy, α - ^{13}C - ^{18}O acid, 4-methyl- (9CI) (CA INDEX NAME)



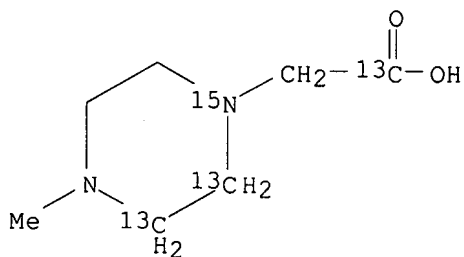
RN 856290-55-6 HCAPLUS

CN 1-Piperazineacetic- α - ^{13}C -1- ^{15}N - ^{18}O acid, 4-methyl- (9CI) (CA INDEX NAME)



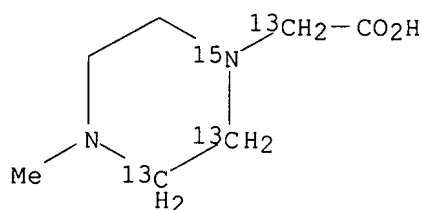
RN 857027-11-3 HCAPLUS

CN 1-Piperazine-2,3- ^{13}C -1- ^{15}N -acetic-carboxy- ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-12-4 HCAPLUS

CN 1-Piperazine-2,3- ^{13}C -1- ^{15}N -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)

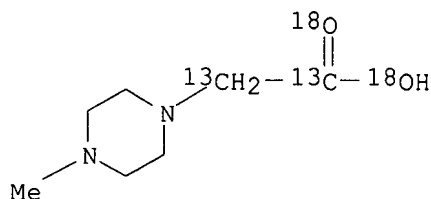


IT 856187-92-3 856188-13-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

RN 856187-92-3 HCAPLUS

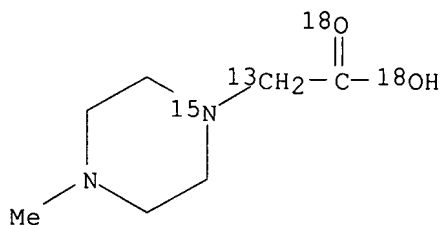
CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ - $^{18}\text{O}_2$ acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

RN 856188-13-1 HCAPLUS

CN 1-Piperazineacetic- α - ^{13}C - ^{15}N - $^{18}\text{O}_2$ acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



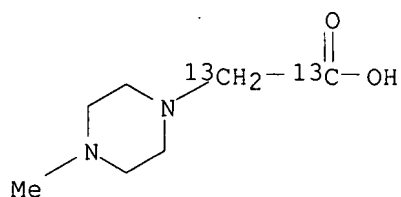
● 2 HCl

IT 856187-68-3P

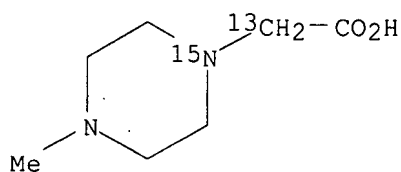
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

RN 856187-68-3 HCAPLUS

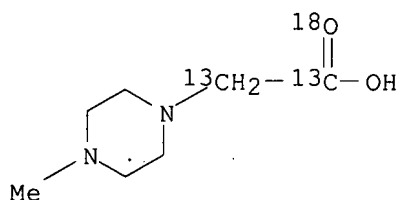
CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ acid, 4-methyl- (9CI) (CA INDEX NAME)



IT **856187-76-3P 857027-06-6DP**, salts
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (mixts. of isobarically labeled analytes and fragments ions derived therefrom)
 RN 856187-76-3 HCAPLUS
 CN 1-Piperazine-1- ^{15}N -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)



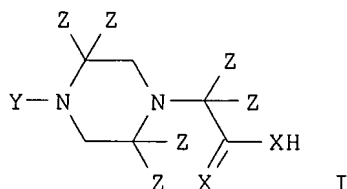
RN 857027-06-6 HCAPLUS
 CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ - ^{18}O acid, 4-methyl- (9CI) (CA INDEX NAME)



L36 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
 AN 2005:588426 HCAPLUS
 DN 143:115568
 TI Preparation of isotopically enriched N-substituted piperazine-1-acetic acids
 IN Dey, Subhakar; Pappin, Darryl J. c.; Purkayastha, Subhasish; Pillai, Sasi; Coull, James M.
 PA Applera Corp., USA
 SO U.S. Pat. Appl. Publ., 29 pp.
 CODEN: USXXCO
 DT Patent
 LA English
 FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005148774	A1	20050707	US 2004-751387	20040105 <--
	AU 2005205522	A1	20050728	AU 2005-205522	20050105 <--
	CA 2552304	A1	20050728	CA 2005-2552304	20050105 <--

WO 2005068446 A1 20050728 WO 2005-US223 20050105 <--
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GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG
EP 1701945 A1 20060920 EP 2005-705033 20050105 <--
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IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS
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US 2004-751354 A 20040105 <--
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US 2004-751388 A 20040105 <--
US 2004-822639 A 20040412
US 2004-852730 A 20040524
WO 2005-US223 W 20050105 <--
OS MARPAT 143:115568
GI



AB Isotopically enriched N-substituted piperazine-1-acetic acids (I) or salts thereof, comprising one or more heavy atom isotopes [X = O, S; Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or F atoms; Z = independently H, deuterium, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms), a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms, or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms)] are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to

label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like. Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-¹³C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on

the

combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-¹³C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-¹³C.

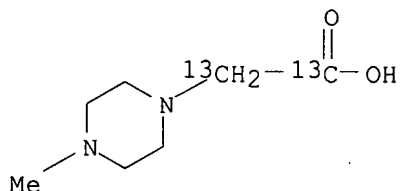
IT **856187-68-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

RN 856187-68-3 HCAPLUS

CN 1-Piperazineacetic-carboxy,α-¹³C2 acid, 4-methyl- (9CI) (CA INDEX NAME)



IT **856187-76-3P 856187-92-3P 856290-53-4P**

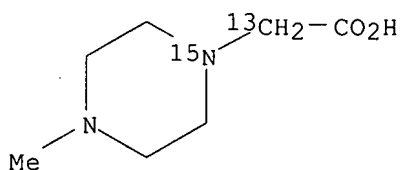
856290-55-6P 857027-11-3P 857027-12-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

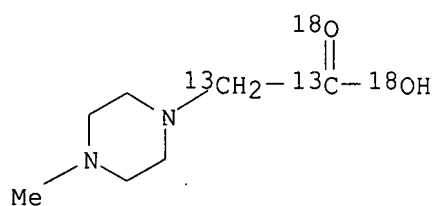
RN 856187-76-3 HCAPLUS

CN 1-Piperazine-1-¹⁵N-acetic-α-¹³C acid, 4-methyl- (9CI) (CA INDEX NAME)



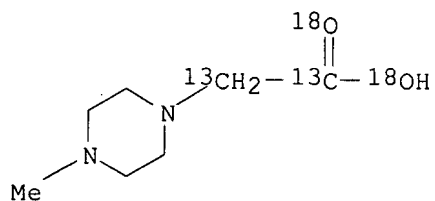
RN 856187-92-3 HCAPLUS

CN 1-Piperazineacetic-carboxy,α-¹³C2-¹⁸O2 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

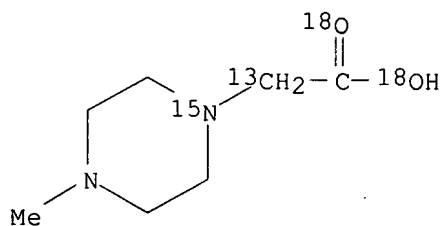


● 2 HCl

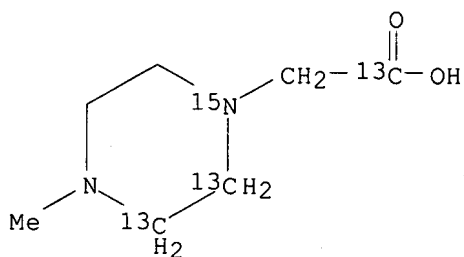
RN 856290-53-4 HCAPLUS
CN 1-Piperazineacetic-carboxy, α -13C2-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856290-55-6 HCAPLUS
CN 1-Piperazineacetic- α -13C-1-15N-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)

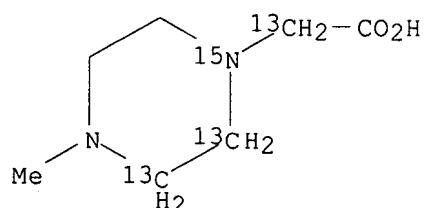


RN 857027-11-3 HCAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-acetic-carboxy-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-12-4 HCAPLUS

CN 1-Piperazine-2,3-¹³C-1-¹⁵N-acetic- α -¹³C acid, 4-methyl- (9CI) (CA
INDEX NAME)



L36 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:588349 HCAPLUS
DN 143:112150
TI Isobarically labeled analytes and fragment ions derived therefrom
IN Pappin, Darryl J. C.; Purkayastha, Subhasish;
Coull, James M.
PA Applera Corporation, USA
SO U.S. Pat. Appl. Publ., 88 pp., Cont.-in-part of U.S. Ser. No. 822,639.
CODEN: USXXCO

DT Patent
LA English

FAN.CNT 6

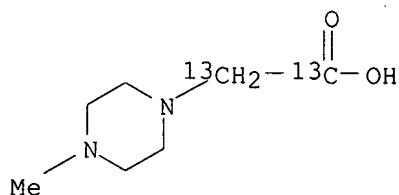
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	MR, NE, SN, TD, TG				
EP	1701945	A1	20060920	EP 2005-705033	20050105 <--
	R:				
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	US 2004-822639	A2	20040412		
	US 2004-751354	A	20040105	<--	
	US 2004-751387	A	20040105	<--	
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	US 2004-852730	A	20040524		
	WO 2005-US223	W	20050105	<--	
OS	MARPAT 143:112150				
AB	This invention pertains to isobarically labeled analytes and fragment ions thereof.				
IT	856187-68-3P 856187-76-3P 856290-53-4P				
	856290-55-6P 857027-06-6P 857291-36-2P				

857291-38-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (isobarically labeled analytes and fragment ions derived therefrom)

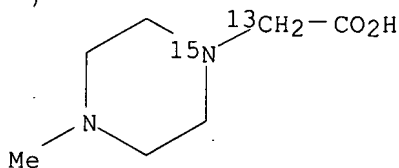
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CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ acid, 4-methyl- (9CI) (CA INDEX NAME)



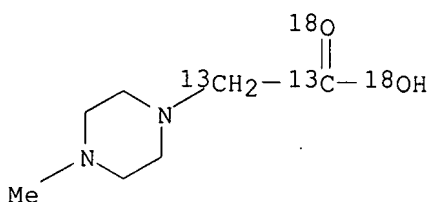
RN 856187-76-3 HCAPLUS

CN 1-Piperazine-1- ^{15}N -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)



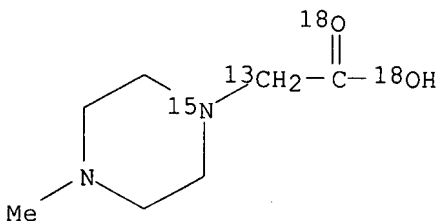
RN 856290-53-4 HCAPLUS

CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}_2$ - $^{18}\text{O}_2$ acid, 4-methyl- (9CI) (CA INDEX NAME)



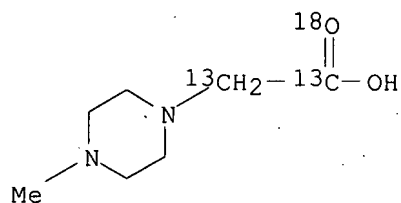
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CN 1-Piperazineacetic- α - ^{13}C -1- ^{15}N - $^{18}\text{O}_2$ acid, 4-methyl- (9CI) (CA INDEX NAME)



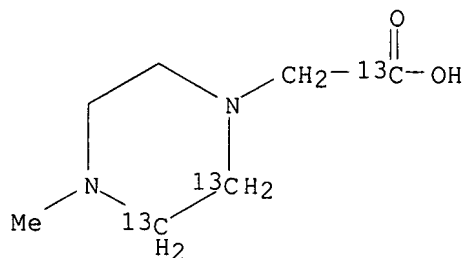
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CN 1-Piperazineacetic-carboxy, α - ^{13}C -180 acid, 4-methyl- (9CI) (CA INDEX NAME)



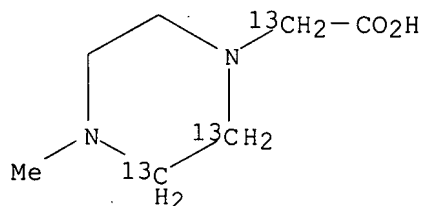
RN 857291-36-2 HCAPLUS

CN 1-Piperazine-2,3- ^{13}C -acetic-carboxy- ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857291-38-4 HCAPLUS

CN 1-Piperazine-2,3- ^{13}C -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)



L36 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:588336 HCAPLUS

DN 143:93635

TI Mixtures of isobarically labeled analytes and fragments ions derived therefrom

IN Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.

PA Applera Corporation, USA

SO U.S. Pat. Appl. Publ., 29 pp.

CODEN: USXXCO

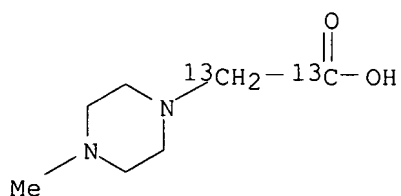
DT Patent

LA English

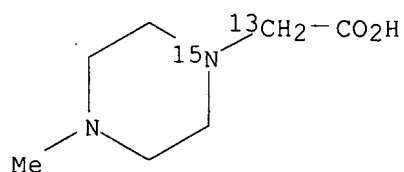
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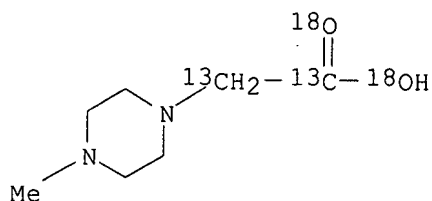
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 US 2004-751388 A 20040105 <--
 US 2004-822639 A2 20040412
 US 2004-852730 A 20040524
 WO 2005-US223 W 20050105 <--
 AB This invention pertains to mixts. of isobarically labeled analytes and
 fragment ions thereof.
 IT **856187-68-3P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (mixts. of isobarically labeled analytes and fragments ions derived
 therefrom)
 RN 856187-68-3 HCAPLUS
 CN 1-Piperazineacetic-carboxy, α - ^{13}C 2 acid, 4-methyl- (9CI) (CA INDEX
 NAME)



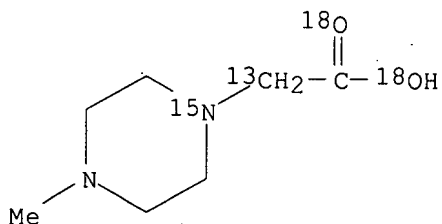
IT **856187-76-3P 856290-53-4P 856290-55-6P**
857027-06-6DP, salts 857027-11-3P 857027-12-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (mixts. of isobarically labeled analytes and fragments ions derived
 therefrom)
 RN 856187-76-3 HCAPLUS
 CN 1-Piperazine-1- ^{15}N -acetic- α - ^{13}C acid, 4-methyl- (9CI) (CA INDEX
 NAME)



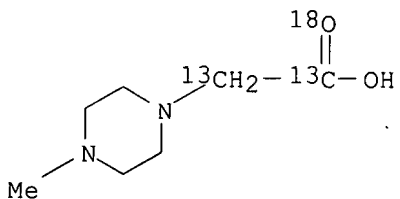
RN 856290-53-4 HCAPLUS
 CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}2$ - $^{18}\text{O}2$ acid, 4-methyl- (9CI) (CA INDEX NAME)



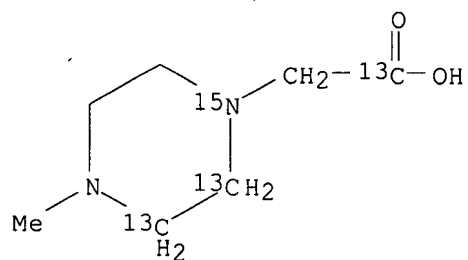
RN 856290-55-6 HCAPLUS
 CN 1-Piperazineacetic- α - ^{13}C -1- ^{15}N - $^{18}\text{O}2$ acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-06-6 HCAPLUS
 CN 1-Piperazineacetic-carboxy, α - $^{13}\text{C}2$ - ^{18}O acid, 4-methyl- (9CI) (CA INDEX NAME)

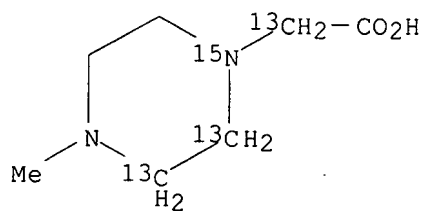


RN 857027-11-3 HCAPLUS
 CN 1-Piperazine-2,3- $^{13}\text{C}2$ -1- ^{15}N -acetic-carboxy- ^{13}C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-12-4 HCAPLUS

CN 1-Piperazine-2,3-¹³C2-1-¹⁵N-acetic- α -¹³C acid, 4-methyl- (9CI) (CA
INDEX NAME)



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